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Effects of pitched tips of novel kneading disks on melt mixing in twin-screw extrusion

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Abstract

In mixing highly viscous materials, like polymers, foods, and rubbers, the geometric structure of the mixing device is a determining factor for the quality of the mixing process. In pitched-tip kneading disks (ptKD), a novel type of mixing element, based on conventional kneading disks (KD), the tip angle is modified to change the channel geometry as well as the drag ability of KD. We discuss the effects of the tip angle in ptKD on mixing characteristics based on numerical simulation of the flow in the melt-mixing zone under different feed rates and a screw rotation speed. It turns out that the passage of fluid through the high-stress regions increases in ptKD compared to conventional KD regardless of the directions and sizes of the tip angle, while the fluctuation in residence time stays at the same level as the conventional KD. Furthermore, pitched tips of backward direction increase the mean applied stress on the fluid elements during its residence in the melt-mixing zone, suggesting the enhancement of dispersive mixing quality in ptKD. These understandings of the role of the tip angle on KD can give a basic guide in selecting and designing suitable angle parameters of ptKD for different mixing purposes.

Keywords: Polymer processing, Mixing, Twin-screw extrusion, Numerical simulation

1. Introduction

Twin-screw devices are widely applied in various industries, including polymer processing, rubber compounding, food processing, and pharmaceutical development, because a high mixing performance can be achieved by the inter-meshing configuration of twin screws.^{1, 2, 3, 4, 5)} In the plastics industry, twin-screw extruders are used to develop polymer materials with certain desired properties by mixing different fillers and additives with polymer melts. For this melt-mixing process, several types of

screw elements have been developed for different material processabilities and different mixing qualities, since the quality of the mixing process is primarily determined by the geometric structure of the mixing element. In selecting and/or developing a mixing element, one fundamental issue is a systematic understanding of the relation between the melt flow driven by the geometric structure of the mixing element and the mixing characteristics.

Among various types of mixing elements,^{6, 7, 8, 9, 10, 11, 12, 13, 14, 15, 16, 17, 18, 19, 5, 20, 21, 22, 23)} kneading disks (KD) are the most commonly used due to their mixing efficiency. In order to tune the mixing characteristics of conventional KD for application to various purposes, a modified type of KD has been proposed, called “pitched-tip kneading disks” (ptKD).²⁴⁾

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In ptKD, two disk tips are pitched to the screw axes, whereas the tips in the conventional KD are parallel to the screw axes. The combined choice of the tip angle and the disk-stagger angle can make it possible to control both the distributive and dispersive mixing abilities better than in conventional KD. In the previous study,²⁴⁾ it has been found that different combinations of tip angle and disk-stagger angle actually lead to different mixing characteristics. Nonetheless, the essential role of the tip angle, specifically its direction and size, on the modification of the flow pattern and the resulting mixing characteristics are still unclear.

In this article, we investigate how pitched tips modify the mixing characteristics of conventional KD in twin-screw extrusion. For this purpose, we consider different directions and sizes of the tip angle on a neutrally staggered KD, and discuss their mixing characteristics using numerical simulation of the polymer-melt flow in the kneading zone.

2. Pitched-tip kneading elements

Conventional kneading disks (KD) are composed of several oval blocks combined with a stagger angle between two adjacent blocks (Fig. 1(c)). The tips of the blocks used in conventional KD are parallel to the screw axes. In contrast to this, in pitched-tip KD, the tips of the blocks are twisted to the screw axes.²⁴⁾ Pitched tips modify the channel geometry of the conventional KD. Furthermore, pitched tips add additional drag ability along with screw rotation to conventional KD. The tip angles associated with forward pump will be called “forward tip” (Ft) and define its tip angle as positive. Conversely, for negative tip angles, pitched tips add backward pump to a block, so that we will call it “backward tip” (Bt). Along with this terminology, we will call the conventional block with zero tip angle the “neutral tip” (Nt).

The typical ptKD has been designed by adjusting both the tip angle and the disk-stagger angle, and therefore its mixing characteristics are determined by the combination of the tip angle and the disk-stagger angle.²⁴⁾ Effects solely due to the pitched tip have not been discussed systematically in previous works. In this paper, we investigate the effects of the pitched tip direction and its angle on the mixing characteristics. For this purpose, ptKDs with a disk-stagger angle and different tip angles, shown

in Fig. 1, are chosen. Based on five-block kneading elements of $L/D = 1.47$ with a disk-stagger angle of 90° , pitched tips with different tip angles from -30° to 30° are arranged.

3. Numerical Simulation

The flow of a polymer melt in the melt-mixing zone of a twin-screw extruder has been numerically solved to allow understanding the relation between the melt-mixing characteristics and the geometry of the kneading elements. The numerical method to study the melt-mixing zone in this paper follows that of the previous paper.²⁴⁾ Here we give a summary of the numerical simulation. We focus on the situation where the material fully fills the channel. The Reynolds number is assumed to be much less than unity, so that inertial effects are neglected. The flow is assumed to be incompressible, and in a pseudo-steady state to screw rotation, as has often been assumed in polymer flow in twin-screw extruders.^{11, 15, 18, 20, 24, 25, 26, 22)} With these assumptions, the governing equations become

$$\nabla \cdot \mathbf{v} = 0, \quad (1)$$

$$\mathbf{0} = -\nabla p + \nabla \cdot \boldsymbol{\tau}, \quad (2)$$

$$\rho C_p \mathbf{v} \cdot \nabla T = k \nabla^2 T + \boldsymbol{\tau} : \mathbf{D}, \quad (3)$$

where \mathbf{v} is the velocity, p is the pressure, $\boldsymbol{\tau}$ is the deviatoric stress, ρ is the mass density, c_p is the specific heat capacity, T is the temperature, k is the thermal conductivity, and $\mathbf{D} = [\nabla \mathbf{v} + (\nabla \mathbf{v})^T]/2$ is the strain-rate tensor, where $(\cdot)^T$ indicates the transpose.

The fluid is assumed to be a viscous shear-thinning fluid that follows Cross-exponential viscosity,²⁷⁾

$$\boldsymbol{\tau} = 2\eta \mathbf{D}, \quad (4)$$

$$\eta(\dot{\gamma}, T) = \frac{\eta_0(T_0)H(T, T_0)}{1 + (\lambda(T_0)H(T, T_0)\dot{\gamma})^{1-n}}, \quad (5)$$

$$H(T, T_0) = \exp[-\beta(T - T_0)], \quad (6)$$

$$\dot{\gamma} = \sqrt{2\mathbf{D} : \mathbf{D}}, \quad (7)$$

whose parameters are obtained by fitting the shear viscosity of a polypropylene melt taken from,¹¹⁾ and the values are $T_0 = 473.15$ K, $\eta_0(T_0) = 32783$ Pa·s, $n = 0.33$, $\beta = 0.0208$ K⁻¹, and $\lambda(T_0) = 1.702$ s. The mass density, specific heat capacity, and thermal conductivity are

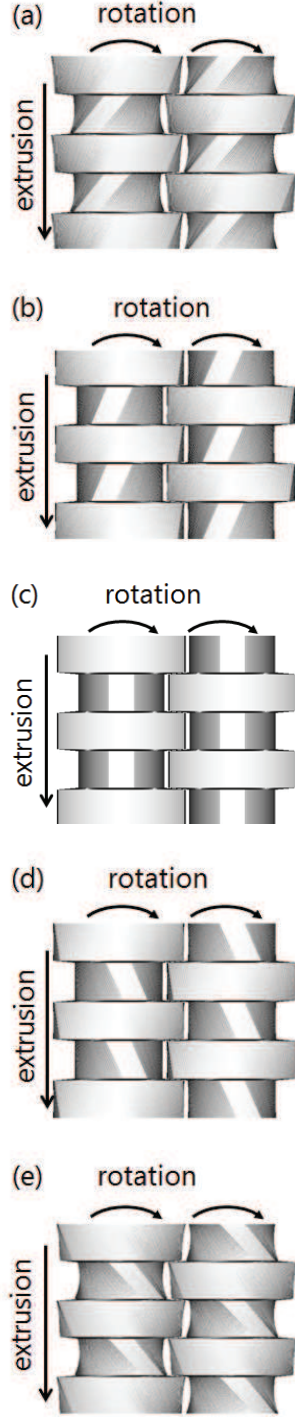


Figure 1: Top view of pitched-tip kneading disks used in this study. Stagger angle of adjacent blocks is set to a value of 90° for all the kneading disks while tip β angle varies from -30° to 30° . (a) forwarding ptKD with a tip angle of 30° (Ft30), (b) forwarding ptKD with a tip angle of 15° (Ft15), (c) conventional KD with a tip angle of 0° (Nt), (d) backwarding ptKD with a tip angle of -15° (Bt15), and (e) backwarding ptKD with a tip angle of -30° (Bt30).

taken from¹¹⁾ as well, and the values are $\rho = 735.0 \text{ kg/m}^3$, $c_p = 2100 \text{ J/(kg}\cdot\text{K)}$, and $k = 0.15 \text{ W/(m}\cdot\text{K)}$.

As operational conditions, the screw rotation speed is set to 200 rpm, while the volume flow rate varies in the range of $5\text{--}120 \text{ cm}^3/\text{s}$ ($\approx 13\text{--}318 \text{ kg/h}$), so that the value of Q/N lies in the range of $1.5\text{--}36 \text{ cm}^3$. The no-slip condition on the velocity at the barrel and screw surfaces is assumed. The velocity at the inlet and outlet boundaries was set to be uniform under the given volumetric flow rate. The pressure at the outlet boundary was fixed to be a constant value. The temperatures on the barrel surface and at the inlet boundary were set to 473.15 K and 453.15 K , respectively. The natural boundary conditions for the temperature equation in the exit boundary plane and the screw surface were assigned. The time evolution of the velocity and temperature fields was constructed with the converged fields for every three degrees of screw rotation.

The trajectories of the passive tracers were determined based on the solved velocity field. The set of tracer trajectories was utilized to compute the residence time distribution^{28,5)} and to investigate the flow history and mixing process. The Lagrangian-history average of a quantity f over the trajectory of α th tracer is defined as

$$\overline{f}_\alpha^{T_\alpha} = \frac{1}{T_\alpha} \int_0^{T_\alpha} ds \int d\mathbf{x} \delta(\mathbf{x} - \mathbf{X}_\alpha(s)) f(\mathbf{x}, s), \quad (8)$$

where T_α and $\mathbf{X}_\alpha(\cdot)$ are the residence time and position of the α th tracer, respectively, and $\delta(\cdot)$ is the Dirac delta distribution. The statistical distribution of $\overline{f}_\alpha^{T_\alpha}$ characterizes the global flow characteristics in the melt-mixing zone.

Initially, 2000 points were uniformly distributed in a certain section relative to the axial position, which was arbitrarily set in the second disk. They were advected until they reached the outlet section. When computing the tracer advection, some tracers went out of bounds because the time resolution of the velocity field was limited. To circumvent the effect of the lost tracers on the statistics, we set the number of initial points to 2000, which ensured that a sufficient number of points reached the outlet.

4. Results and Discussion

In order to see the effect of the tip angle on the inhomogeneity of cross-sectional mixing, we computed the fluctuation of the residence time. Figure 2 shows the

probability density of the residence time normalized by the mean residence time for five different ptKDs under $Q/N = 9 \text{ cm}^3$. From this figure, we observe that the residence time distribution is almost unaffected by the forward tip angle while the fraction of the longer residence increases with a backward tip angle. In Fig. 3, there is drawn the relative standard deviation of the residence time to its mean value as a function of Q/N . It turns out that the fluctuation of the residence time in ptKDs hardly depends on Q/N , and takes the value of 0.5–0.6. At higher values of Q/N , the residence time fluctuation is approximately the same level as that of the conventional KD. This fact suggests that ptKDs have as good mixing ability as the conventional KD with the same disk-stagger angle at sufficiently high Q/N .

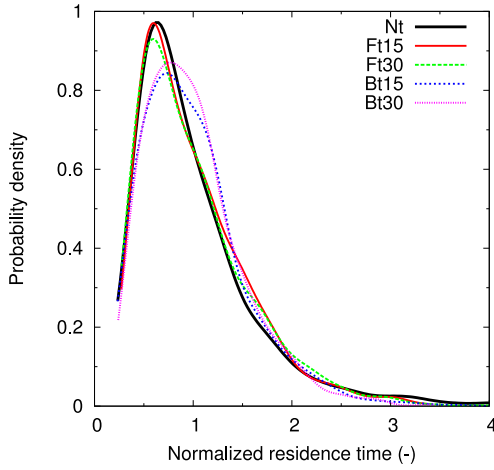


Figure 2: Normalized residence time distribution for Ft30, Ft15, Nt, Bt15, and Bt30 under $Q/N = 9 \text{ cm}^3$. Residence time is normalized by the mean residence time.

The effect of the tip angle on the residence time distribution depends on the tip direction. While for Ft type the residence time fluctuation does not show any angle-dependence, for Bt type the residence time fluctuation decreases slightly with the backward tip angle. Although this slight change of residence time fluctuation reflects the effect of the tip angle, this change does not seem to be substantial in terms of mixing ability. In short, the residence time distribution is not substantially modified by the addition of a tip angle to a conventional KD.

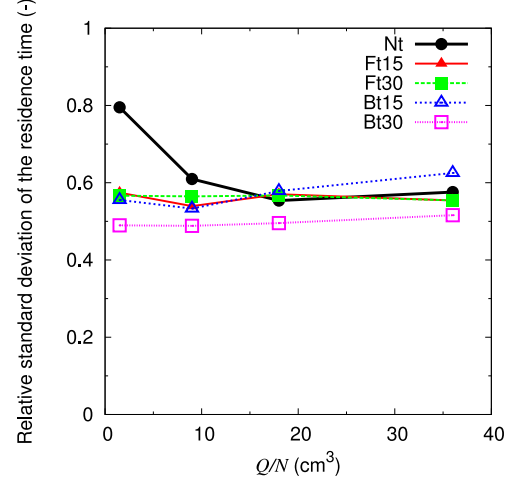


Figure 3: Relative standard deviation of the residence time to its mean value as a function of Q/N for Ft30, Ft15, Nt, Bt15, and Bt30.

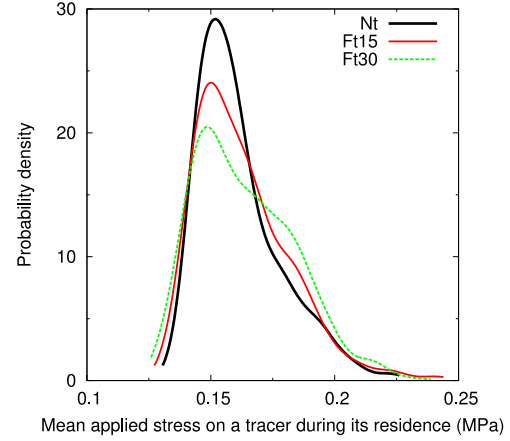


Figure 4: Probability density function of the applied stress during residence, $\overline{\sigma}_\alpha^{T_\alpha}$, for Ft30, Ft15, and Nt under $Q/N = 9 \text{ cm}^3$.

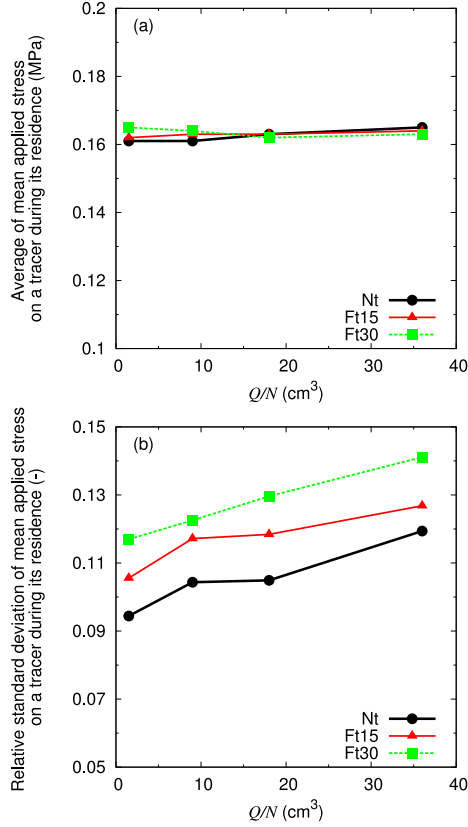


Figure 5: (a) Average value and (b) the relative standard deviation of $\overline{\sigma}_\alpha^{T_\alpha}$ as a function of Q/N for Ft30, Ft15, and Nt.

Next, we discuss the effects of a pitched tip on dispersive mixing. The mean applied stress during residence, $\overline{\sigma}_\alpha^{T_\alpha}$, is calculated by inserting the stress magnitude $\sigma = \sqrt{(3/2)\tau} : \tau$ into Eq. (8). Figure 4 shows the probability density function of $\overline{\sigma}_\alpha^{T_\alpha}$ for Ft15, Ft30, and Nt under $Q/N = 9$ cm³. As the forward tip angle increases, the fluctuation of $\overline{\sigma}_\alpha^{T_\alpha}$ increases, whereas the average of $\overline{\sigma}_\alpha^{T_\alpha}$ stays at a similar level as that of Nt. The average value and the relative standard deviation of $\overline{\sigma}_\alpha^{T_\alpha}$ as a function of Q/N are drawn in Figs. 5(a) and (b), respectively. The average value of $\overline{\sigma}_\alpha^{T_\alpha}$ is insensitive to Q/N , and takes a similar value as that of Nt. In contrast, the fluctuation of $\overline{\sigma}_\alpha^{T_\alpha}$ increases with Q/N , and is larger for a larger forward tip angle. These results clearly indicate that the forward tip increases the inhomogeneity of dispersive mixing quality especially at high throughput operation.

Figure 6 shows the probability density function of $\overline{\sigma}_\alpha^{T_\alpha}$ for Bt15, Bt30, and Nt under $Q/N = 9$ cm³. In Fig. 6, we observe an increase both in the average level and the fluctuation of $\overline{\sigma}_\alpha^{T_\alpha}$ with an increase in the backward tip angle. The average value and the relative standard deviation of $\overline{\sigma}_\alpha^{T_\alpha}$ as a function of Q/N are drawn in Figs. 7(a) and (b), respectively. In Fig. 7, the average value of $\overline{\sigma}_\alpha^{T_\alpha}$ becomes larger for a larger backward tip angle, suggesting that the Bt type enhances the dispersive mixing ability compared to the Nt type. In contrast, the fluctuation of $\overline{\sigma}_\alpha^{T_\alpha}$ is rather insensitive to the backward tip angle. That is, irrespective of Bt angle, the inhomogeneity of the dispersive mixing is at the same level as that of the Nt type. With an increase of Q/N , the fluctuation of $\overline{\sigma}_\alpha^{T_\alpha}$ for Bt slightly increases, suggesting that inhomogeneity in the dispersive mixing is smaller for lower Q/N . In short, for Bt type, both high level and small inhomogeneity of $\overline{\sigma}_\alpha^{T_\alpha}$ is achieved at low Q/N conditions, indicating that that dispersive mixing in Bt type is most effective when Q/N is low and the Bt angle is large.

In order to further study the effects of the tip-angle on dispersive mixing, the passage of fluid at high-stress regions has been investigated. Irrespective of the tip angle, the highest shear stress is achieved in the small gap regions like the tip-barrel clearance and the inter-meshing region. The substantial dispersion process mainly takes place when fluid elements pass through such high-stress regions. However, since the high-stress region occupies only a small fraction of the whole channel, the fraction

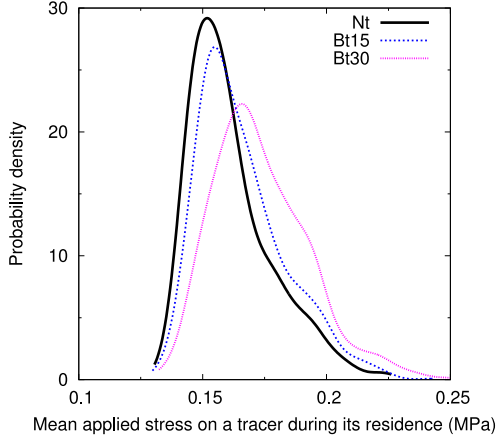


Figure 6: Probability density function of the applied stress during residence, $\overline{\sigma_\alpha}^{T_\alpha}$, for Bt30, Bt15, and Nt under $Q/N = 9 \text{ cm}^3$.

of the fluid passing through these regions and the number of passages are essentially determined by the flow pattern at the low-stress (low-shear-rate) regions. Thus, the geometric structures of the mixing elements are directly responsible for the passage of fluid through the high-stress regions, eventually leading to a better dispersive mixing performance.

By setting a threshold value for the magnitude of the shear stress tensor, the regions of tip-barrel clearance and the screw inter-meshing region are defined as the high-stress regions. For instance, the region where the shear stress magnitude is larger than 0.35 MPa for Nt type under $Q/N = 18 \text{ cm}^3$ is shown in Fig. 8, which clearly shows that the high-stress region is localized at around tip-clearance and inter-meshing regions. We calculated the fraction of the tracers passing through the high-stress regions as well as the residence time in those regions.

For each tracer, the residence time in the high-stress regions, $t_{h,\alpha}$, as well as the residence time in the whole mixing zone, T_α , has been studied. Figures 9(a) and (b) show the probability density function of the ratio $t_{h,\alpha}/T_\alpha$ under $Q/N = 9 \text{ cm}^3$. At a first look at Figs. 9(a) and (b), the residence time in the high-stress regions is at most 0.1 during the residence in whole zone, irrespective of the tip angle. Both for Ft and Bt types, the residence in the high-stress regions becomes longer compared to the Nt type, indicating that the pitched-tip geometry can enhance the

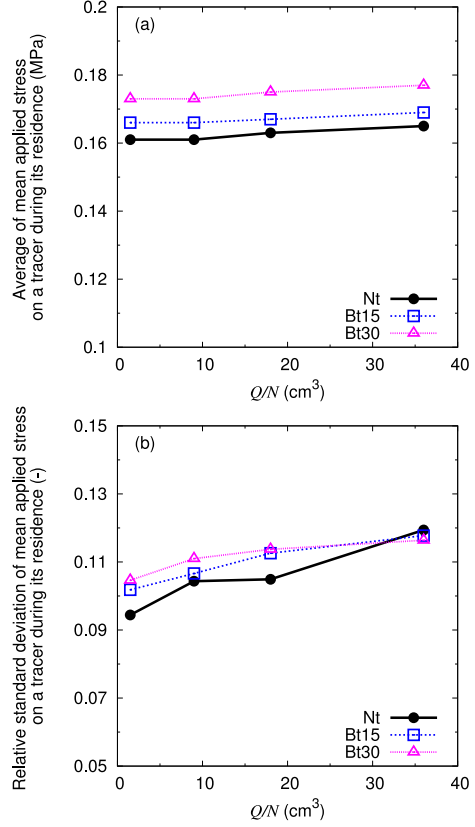


Figure 7: (a) Average value and (b) the relative standard deviation of $\overline{\sigma_\alpha}^{T_\alpha}$ as a function of Q/N for Bt30, Bt15, and Nt.

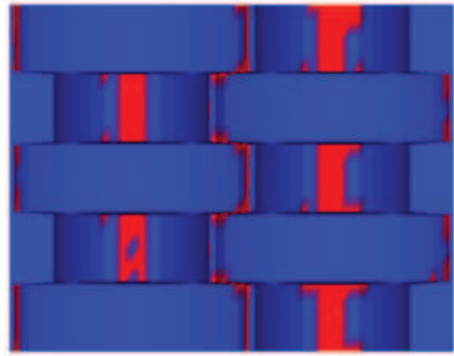


Figure 8: High-stress region for Nt type under $Q/N = 18 \text{ cm}^3$ is drawn in red. In this case, the threshold value of the shear stress magnitude, σ , is arbitrarily set to 0.35 MPa.

efficiency of conveying the fluid to the high-stress regions. The increase of the relative residence in the high-stress regions is more pronounced with the Bt type. This observation partly explains the enhancement of the dispersive mixing by the pitched tip.

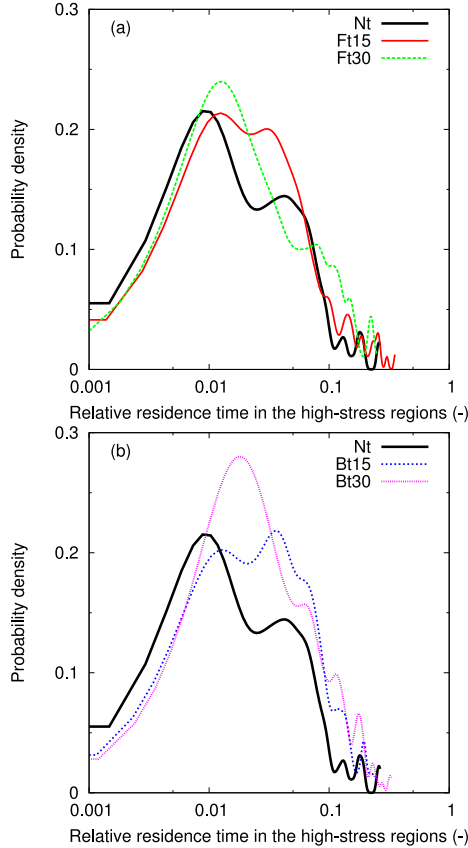


Figure 9: Probability density function of the ratio of the residence time in the high-stress regions to the overall residence time, $t_{h,\alpha}/T_\alpha$, under $Q/N = 9 \text{ cm}^3$: (a) for Ft30, Ft15, and Nt, and (b) for Bt30, Bt15, and Nt.

From Figs. 9(a) and (b), we also observe that the probability of vanishing $t_{h,\alpha}$ takes a finite value, indicating that not all the fluid elements pass through the high-stress regions. In order to study this aspect, we discuss the fraction of the tracers passing the high-stress regions, denoted by Φ . In Figs. 10(a) and (b), Φ is plotted to the mean residence time of high-stress regions, $\langle t_h \rangle$, for different Q/N values, in which the larger symbol is for the larger value of

Q/N . In the plot of Φ_h and $\langle t_h \rangle$, the upper locations means that a large fraction of tracers pass through the high-stress regions, while the right locations means that the tracers stay long time in the high-stress regions. Hence, the upper and right locations indicate a high potential for dispersive mixing.

For conventional Nt type, a fraction, 0.4–0.5, of the fluid passes through the high-stress region for the Q/N value studied. Furthermore, Φ_h and $\langle t_h \rangle$ are rather insensitive to the value of Q/N . In contrast, for Ft and Bt types, Φ_h and $\langle t_h \rangle$ show a relatively large dependence on Q/N . We observe a general trend such that, as Q/N decreases, both Φ_h and $\langle t_h \rangle$ increase. In addition, the characteristics of the passage through the high-stress region have different tip-angle dependencies with different directions of the tip angle. While for Ft type, Φ_h and $\langle t_h \rangle$ does not depend on the tip angle, for Bt type, Φ_h and $\langle t_h \rangle$ take larger values for larger backward tip angles. This fact is consistent with the tip-angle dependence of the mean applied stress during residence in Fig. 5(a) and 7(a). The characteristics of the passage through the high-stress region reveal that the backward tip is effective at enhancing the dispersive mixing ability.

From the data above, it turns out that the pitched tip modifies the dispersive mixing ability of kneading disks, and the backward tip enhanced the potential of dispersive mixing while keeping the distributive mixing ability. We discuss the relation between the flow pattern induced by the geometry of the pitched-tip KD and the dispersive mixing ability. Pitched tips add an additional drag ability along the screw rotation to conventional KD. For backward tips increase the drag in the backward extrusion direction, for $Q > 0$ condition, the pressure drop in Bt type becomes larger than that in Nt, leading to the pressure flow in the extrusion direction being more pronounced in Bt. The enhanced pressure flow in Bt promotes the passage of fluid across the small gap at the backward tips, resulting in an increase of the passage through the high-stress regions and the mean applied stress. In other words, the geometry of backward tips cause a counteracting effect by blocking against the forward flow and the additional forward pressure flow while keeping the leakage flow in the inter-disk spaces. Since this effect is driven by the screw rotation, it is maximized with the small Q/N condition, which is clearly demonstrated by the characteristics of the passage through the high-stress region in

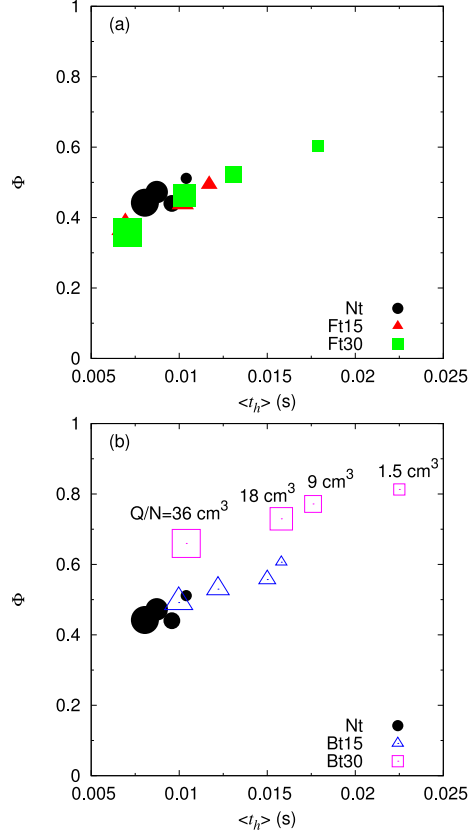


Figure 10: Fraction of the tracers passing through the high-stress regions, Φ , and the mean residence time in those regions, $\langle t_h \rangle$, for different values of $Q/N = 1.5, 9, 18$, and 36 cm^3 : (a) for Ft30, Ft15, and Nt, and (b) for Bt30, Bt15, and Nt. The larger symbol is for the larger value of Q/N .

Fig. 10.

In the case of Ft type, since the forward pitched tips increase the drag in the forward direction, for $Q > 0$ conditions the pressure drop become smaller than for Nt, or even becomes negative, depending on Q/N . Thus, the counteracting effect of the pressure flow and the blockage by the tips is weaker in the Ft type than in the Bt type.

In short, the geometric modification of conventional KD by pitched tips induces both a change in the channel geometry and a modification of the pressure flow, causing a change in dispersive mixing ability.

5. Conclusions

In pitched-tip kneading disks (ptKD), a novel melt-mixing element used in twin-screw extrusion, the effects of the direction and size of the tip angle on the mixing characteristics were investigated based on the numerical simulation of a three-dimensional flow. Under a material feed rate and a screw rotation speed, the tip angle on a conventional kneading-disk (KD) element modifies the following two properties of the flow: (i) additional drag ability caused by screw rotation modifies the pressure flow, (ii) the pitched-tip acts as a blockage to the pressure flow induced by the pitched-tip. These counteracting effects result in an increase of the fraction of the fluid elements passing through the high-stress regions, leading to a modification of the dispersive mixing ability.

Forward tips on neutrally staggered KD increase the inhomogeneity of the applied stress during residence compared to the conventional KD, while keeping the residence time fluctuation. In contrast, backward tips on neutrally staggered KD increase the mean applied stress during residence, suggesting an enhancement of the dispersive mixing ability. These effects are more pronounced for larger tip angles, and are dependent on the ratio of the material feed rate to the screw rotation speed. These findings about the role of the tip angle can be useful for a better understanding of the mixing characteristics of a general class of ptKD elements and for choosing the optimal combination of the disk-stagger angle and tip angle.

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